Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.45

Global applicability domain: Inside

Local applicability domain index: 5.25e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

Image not found
1,2-Dichlorobenzene
Measured: 3.43
Predicted: 2.45

Image not found
Ethanone, 1-(2-thienyl)-
Measured: 1.25
Predicted: 1.86

Image not found
Thiophene, 3-methyl-
Measured: 2.34
Predicted: 2.35

Image not found
Pyridine, 2,3,5-trichloro-
Measured: 3.11
Predicted: 2.61

Image not found
1,4-Dichloro-2-butyne
Measured: 2.01
Predicted: 2.05